Transition from particlelike to wavelike behavior for an electron in one-dimensional nonuniform lattice systems

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We explore a distinguishability D and a visibility V, satisfying the relation $D^2 + V^2 = 1$, to measure a single electron's particlelike and wavelike behaviors, respectively. For several typical one-dimensional nonuniform lattice systems, we find that D^2 is less than, equal to, and greater than V^2 for delocalized, critical, and localized states, respectively. In this sense, the Anderson transition can be viewed as a transition from relatively more particlelike behavior to relatively more wavelike behavior.

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I. INTRODUCTION

An electron moving in a lattice system may exhibit fully particlelike behavior if it is completely localized at a site or fully wavelike behavior if it is uniformly distributed at all sites. However, it is generally in intermediate states and it has both particlelike and wavelike properties, i.e., the wave-particle duality. For a long time, many works have focused on the transition from particlelike behavior to wavelike behavior [1–3].

In fact, the wave-particle duality is embodied in Bohr's principle of complementarity [4]. Though the two different properties cannot be simultaneously observed or measured, to some extent this duality can be mathematically evaluated by some uncertainty relations, e.g., the Heisenberg uncertainty relation [5–7], the entropic uncertainty relation [8–10], and some novel uncertainty relations [11,12]. For the Heisenberg uncertainty relation, formulated as $\Delta x \Delta p \geqslant \hbar/2$, the relatively smaller is Δx, the relatively more particlelike behavior a quanton exhibits. However, in some cases both Δx and Δp may be relatively smaller or larger. Therefore, we cannot compare two quantons' particlelike or wavelike properties. Recently, in the context of interferometry, the well-known inequality that $D^2 + V^2 \leqslant 1$ was found to quantify the wave-particle duality, where D is the path distinguishability (particle nature) or which-path information and V is the visibility (wave nature) of the interference pattern behind the interferometer [13–15]. Fortunately, the equality that $D^2 + V^2 = 1$ holds for pure states [13–15]. In this situation, it is easier to compare one quanton's particlelike or wavelike properties to the other quanton's corresponding properties. Subsequently, extensive efforts have been devoted to the study of this wave-particle duality [16–19].

On the other hand, it is well known that Anderson localization is one of the most important and interesting phenomena in solid-state physics, which predicts electron localization in disordered (lattice) systems [20,21]. Moreover, this phenomenon has also been observed in many branches of physics, such as in light waves, sound waves, and matter waves [21]. For electron systems, Anderson transitions, i.e., metal-insulator transitions or delocalization-localization transitions, have received the most attention [21–26]. Historically, electron states without electron-electron interaction in some famous one-dimensional (1D) models have been extensively studied. For example, there are only localized states in the 1D Anderson model with uncorrelated random potential, and there is no mobility edge (ME) separating localized and extended states [27,28]. All states are extended, critical, or localized in the 1D Harper model, depending on the potential strength [29–32]. MEs have been found in the 1D slowly varying potential (SVP) model [33–35]. Although almost all works support these conclusions, some controversial arguments exist. For instance, in the Harper model, a gradual transition from extended to localized states is found in a potential zone near the critical potential [36], and MEs may also exist [37–39]. For the SVP model, power-law decaying states appear close to the ME on the metallic side [40]. Therefore, it is worthwhile to develop new techniques to understand the localization properties in these models.

In this work, inspired by the distinguishability D and the visibility V that characterize the wave-particle duality of a photon in interferometers, we develop two similar quantities to quantify particlelike and wavelike behaviors of a single electron in 1D lattice systems. The results state that the transition from particlelike to wavelike behavior is related to the Anderson transition. At the same time, these studies provide additional evidence supporting the corresponding controversial arguments.

The rest of the paper is organized as follows. In Sec. II, we introduce the distinguishability D and the visibility V in 1D single-electron lattice systems. In Sec. III, we analyze D and V in the Anderson, the Harper, and the SVP models, respectively. Finally, we give a summary of our main results.

II. DISTINGUISHABILITY AND VISIBILITY IN SINGLE-ELECTRON LATTICE SYSTEMS

Generally, for a single electron in 1D lattice systems, the corresponding tight-binding Hamiltonian can be described

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by

$$H = \sum_{i=1}^{N} \varepsilon_i c_i^\dagger c_i - t \sum_{i=1}^{N} (c_i^\dagger c_{i+1} + \text{H.c.}), \tag{1}$$

where ε_i is the on-site potential and t is a nearest-neighbor hopping integral and can be taken to 1 without loss of generality. $c_i^\dagger$ (c_i) is the creation (annihilation) operator at the ith site, and N is the lattice size. The general wave function, i.e., eigenstate $|\beta\rangle$ with eigenenergy E_β for the Hamiltonian in Eq. (1) can be written as the superposition

$$|\beta\rangle = \sum_{i=1}^{N} \phi_i^\beta |i\rangle = \sum_{i=1}^{N} \phi_i^\beta c_i^\dagger |0\rangle, \tag{2}$$

where $|0\rangle$ is the vacuum and ϕ_i^β is the amplitude of the βth wave function at the ith site.

Before we introduce the distinguishability D and the visibility V for a single electron in 1D lattice systems, we first recall them for a single photon in two-path interferometers [16–19]. The two-path superposition state of photons inside the interferometer is

$$\Psi_{1,2} = \psi_1 a_1^\dagger |0\rangle + \psi_2 a_2^\dagger |0\rangle, \tag{3}$$

where $a_k^\dagger$ denotes the creation operators of the modes in path k, and ψ_k is the corresponding amplitude. The operator of distinguishability is given by [19]

$$\hat{D}_{1,2} = \frac{a_1^\dagger a_1 - a_2^\dagger a_2}{\langle a_1^\dagger a_1 \rangle + \langle a_2^\dagger a_2 \rangle}, \tag{4}$$

and that for visibility is given by

$$\hat{V'}_{1,2} = \frac{a_1^\dagger a_2 e^{i\theta} + a_2^\dagger a_1 e^{-i\theta}}{\langle a_1^\dagger a_1 \rangle + \langle a_2^\dagger a_2 \rangle}, \tag{5}$$

where a_k denotes the annihilation operators of the modes in path k, the phase parameter θ is controlled by the phase shifter in the interferometer, and the denominator is for normalization. The two expectation values can be calculated, i.e., the distinguishability $D_{1,2} = |\langle \hat{D}_{1,2} \rangle|$ and the visibility $V_{1,2} = |\langle \hat{V'}_{1,2} \rangle|_{\max \text{ by } \theta}$. Here, $V_{1,2}$ is the maximal value of $\hat{V'}_{1,2}$ at a proper θ. $D_{1,2}$ and $V_{1,2}$ are used to quantify the particlelike information and wavelike informations, respectively. For pure states, the equality that $D_{1,2}^2 + V_{1,2}^2 = 1$ holds.

To adapt $D_{1,2}$ and $V_{1,2}$ for electrons, we straightly map paths 1 and 2 for a photon in the interferometer to sites i and j for an electron in lattice systems, respectively. The corresponding $a_1^\dagger(a_1) \longmapsto c_i^\dagger(c_i)$ and $a_2^\dagger(a_2) \longmapsto c_j^\dagger(c_j)$. Therefore, with Eqs. (4) and (5) and eigenstate $|\beta\rangle$ for an electron in Eq. (2), the local distinguishability $D_{i,j}$ and visibility $V_{i,j}$ between two sites, i and j, can be calculated. For nonuniform systems, the value of $D_{i,j}$ ($V_{i,j}$) depends on sites i and j. For eigenstate $|\beta\rangle$, we define a site-averaged distinguishability squared,

$$D^2 = \frac{2}{N(N-1)} \sum_{i,j(i<j)}^{N} D_{i,j}^2, \tag{6}$$

and a site-averaged visibility squared,

$$V^2 = \frac{2}{N(N-1)} \sum_{i,j(i<j)}^{N} V_{i,j}^2. \tag{7}$$

As we focus on D^2 and V^2 in the rest of the paper, henceforth, we omit "site-averaged" and "squared" for simplicity. To demonstrate Eqs. (6) and (7) intuitively, we give three examples. For a localized state where $\phi_i^\beta = \delta_{ii_0}$ (i_0 is a given site), $D^2 = 1$ and $V^2 = 0$; i.e., it exhibits fully particlelike behavior. For an extended state where $\phi_i^\beta = \frac{1}{\sqrt{N}}$ for all i, $D^2 = 0$ and $V^2 = 1$; i.e., it exhibits fully wavelike behavior. For the two cases, the values of D^2 and V^2 are independent of the lattice sizes. For an extended state where $\phi_i^\beta \propto \sin(ki)$ and $k = 2\pi/N$, $D^2 = 0.363\,745\,89\ldots, 0.363\,416\,58\ldots$, and $0.36338204\ldots$ at $N = 10^3, 10^4$, and 2×10^5, respectively. In the finite-size analysis, $D^2 = 0.363\,379\,91\ldots$ as $N \longrightarrow \infty$. Though its value depends on the lattice sizes, $D^2 < V^2$ always holds for extended states, where $V^2 = 1 - D^2$.

III. RESULTS

In what follows, we study the distinguishability D^2 and visibility V^2 in the Anderson, the Harper, and the SVP models, respectively. In numerical calculations, we directly diagonalize the Hamiltonian in Eq. (1) with the periodic boundary condition to find all eigenenergies E_β and the corresponding eigenstates $|\beta\rangle$. For all these numerical results, the relation $D^2 + V^2 = 1$ always holds and we do not mention it unless necessary.

A. Anderson model

For the 1D Anderson model, the on-site potential ε_i in Eq. (1) is a random variable uniformly chosen within the region $[-W/2, W/2]$, where W characterizes the strength of the disordered potential [20]. It is known that all the eigenstates are localized [27,28]. The average one-particle localization length can be approximately $\xi \sim 105t^2/W^2$ for energy at the band center [23].

Eigenstates with eigenenergies $E_\beta \in [-0.001, 0.001]$ are considered. We plot the spectrum-averaged distinguishability D^2 and visibility V^2 in Fig. 1(a) for lattice sizes $N = 1000$, 3000, and 4500, respectively. Enough disorder realizations have been taken. It shows that for a fixed lattice size N, D^2 increases with disordered potential strength W, while V^2 decreases with W. There is a crossover at a relatively smaller W_{cr} between the two curves for D^2 and V^2 versus W, where $D^2 = V^2 = 0.5$. The larger is N, the smaller W_{cr} is. This is a finite-size effect. For this, we define a reduced localization length $\xi_r = \xi/N$ for every W. We plot D^2 and V^2 versus ξ_r in Fig. 1(b). It shows that the date of D^2 (V^2) obtained from different lattice sizes collapse roughly onto a single curve. The two curves for D^2 and V^2 cross over at $\xi_r^{\text{cr}} \approx 1.6$, i.e., the localization length ξ is of the same order as the system size N. In this case, electrons occupy almost the whole space and thus the system is "metallic." We find that $D^2 > V^2$ when $\xi_r < \xi_r^{\text{cr}}$, while $D^2 < V^2$ when $\xi_r > \xi_r^{\text{cr}}$. This means that particlelike properties are larger than wavelike ones for "insulated" regions, and vice versa for metallic regions.

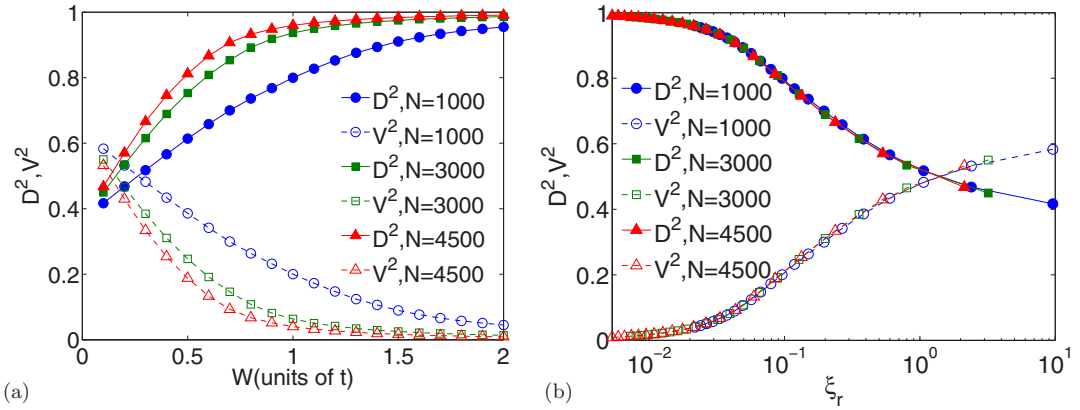

FIG. 1. For the Anderson model, (a) D^2 (filled symbols) and V^2 (open symbols) as functions of W, and (b) D^2 (filled symbols) and V^2 (open symbols) as functions of the corresponding ξ_r, respectively.

B. Harper model

For the Harper model [29–32], the on-site potential in Eq. (1) can be taken by $\varepsilon_i = \lambda \cos(2\pi\sigma i)$, where σ is an irrational number. In our calculations, we choose $\sigma = F_{m-1}/F_m$ and lattice size $N = F_m$, where the Fibonacci numbers $F_m = F_{m-1} + F_{m-2}$. Thus, the periodic approximant can be obtained for the quasiperiodic potential. Almost all works support the conclusions [29–32] that all eigenstates are extended for $\lambda < 2$ but localized for $\lambda > 2$. The metal-insulator transition occurs at $\lambda_c = 2$. However, some studies take different perspectives

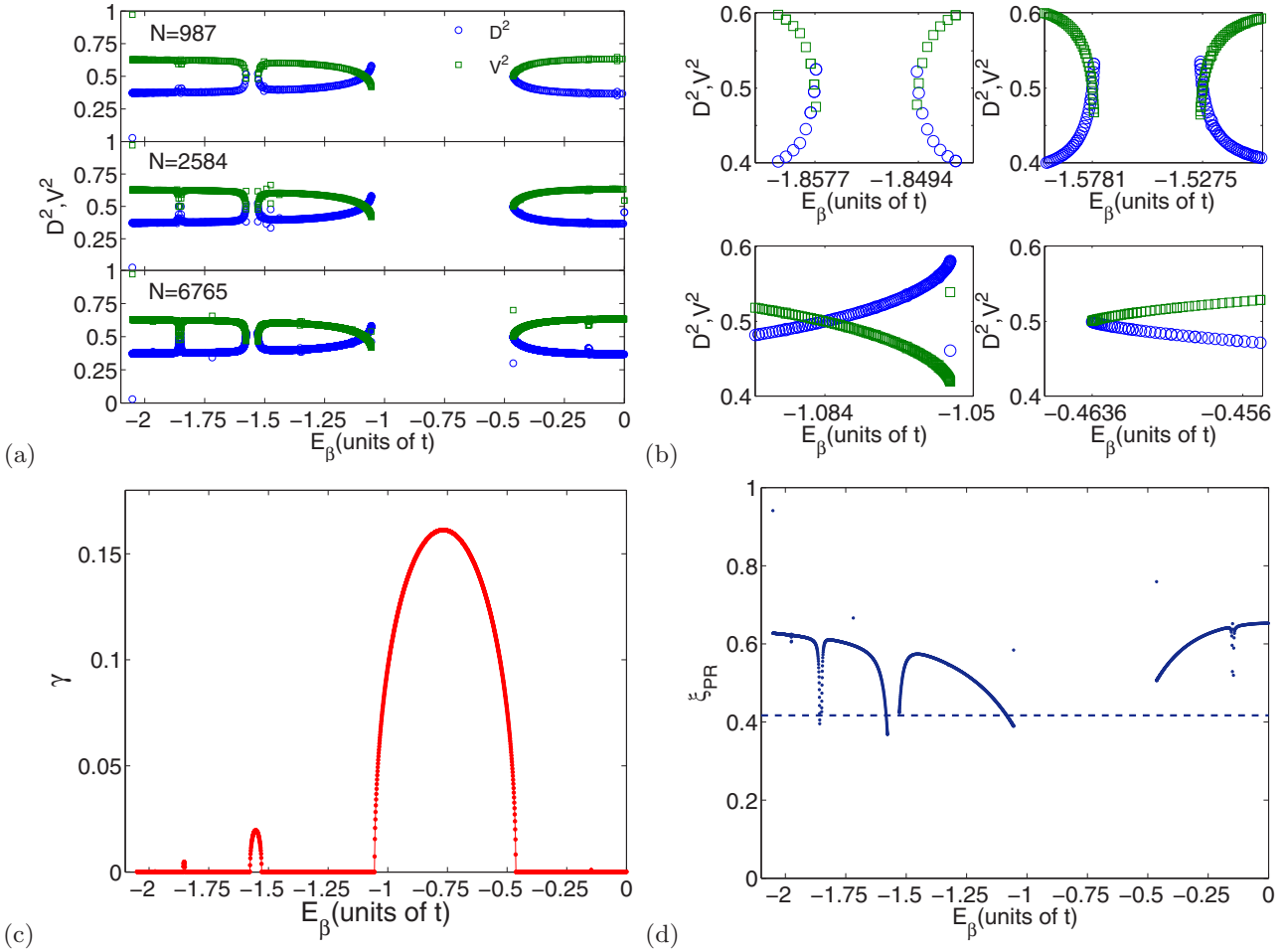

FIG. 2. Some quantities for the Harper model at $\lambda = 0.6$. (a) D^2 (blue symbols) and V^2 (green symbols) as functions of E_β at lattice sizes $N = 987$, 2584, and 6765, respectively. (b) Partial enlarger at the crossover points of D^2 and V^2 in (a) for $N = 6765$. (c) The corresponding γ versus E_β. (d) The corresponding $\xi_{\rm PR}$ versus E_β; the line is for the function $\xi_{\rm PR} = 0.4169$. The lattice size $N = 6765$ for (c) and (d). Due to symmetry, only the E_β half is shown.

[36–39]. For example, Sun and Wang found a gradual transition from extended to localized states when λ is near λ_c; i.e., localized states may exist when $\lambda < \lambda_c$ [36]. Few other groups have discussed the possibility that MEs may exist when $\lambda < \lambda_c$ [37–39].

We take $\lambda = 0.6$ as an example. Some related quantities are plotted in Fig. 2. In detail, Fig. 2(a) shows the variation of the distinguishability D^2 and visibility V^2 with eigenenergies E_β. Here, lattice sizes $N = 987$, 2584, and 6765 are used as examples. They show that $D^2 < V^2$ in some energy regions and $D^2 > V^2$ in others. According to our discussion of the Anderson model in Sec. III A the states are localized when $D^2 > V^2$; i.e., localized states exist when $\lambda < \lambda_c$. Due to the finite-size effect, the relation that $D^2 < V^2$ for some states (for example, E_β is near -1.8577) becomes $D^2 > V^2$ as the lattice size increases. In other words, they are "extended" at relatively smaller lattice sizes, while they are localized at relatively larger ones. For $N = 6765$, a partial enlarger at the crossover points of D^2 and V^2 is plotted in Fig. 2(b). The crossover points correspond to MEs.

To compare the result from D^2 and V^2 with that from traditional quantities, we study the Thouless exponent [22] and the participation ratio [23], which are given by $\gamma(E) = \frac{1}{N}\sum_{\beta, E\neq E_\beta} \ln|E_\beta - E|$ and $\mathrm{PR} = \frac{(\sum_i \phi_i^2)^2}{N\sum_i \phi_i^4}$, respectively. We define the inverse participation ratio $\xi_{\mathrm{PR}} = 1/\mathrm{PR}$. It is known that γ (PR) is proportional to the inverse of the localization length. The corresponding results are plotted in Figs. 2(c) and 2(d), respectively. There, $N = 6765$ is used as an example and the results are similar for larger lattice sizes. The line in Fig 2(d) represents the function $\xi^*_{\mathrm{PR}} = 0.4169$, which is the mean values of all ξ_{PR} at the crossover points in Fig. 2(a). We find that on the whole, γ is near 0 and ξ_{PR} is relatively larger for states with $D^2 < V^2$, while γ is greater than 0 and ξ_{PR} is relatively smaller for states with $D^2 > V^2$. Therefore, our results are consistent with the findings [37–39] that MEs may exist when $\lambda < \lambda_c = 2$. The values of the MEs in Fig. 2 are consistent with those obtained by theoretical and numerical analysis in Ref. [39]. We also have studied D^2 and V^2 for $\lambda > \lambda_c$ and find that $D^2 > V^2$ for all states, which means that they are all localized. Therefore, from all these studies, we can conclude that D^2 is less than, equal to, and greater than V^2 for delocalized, critical, and localized states, respectively.

C. Slowly varying potential model

For the SVP model, the on-site potential in Eq. (1) can be written as $\varepsilon_i = \lambda\cos(\pi\alpha i^\upsilon)$, where λ, α, and $0 \leqslant \upsilon \leqslant 1$ are positive numbers which completely define the tight-binding problem [33–35]. For $0 < \upsilon < 1$, there are two MEs at

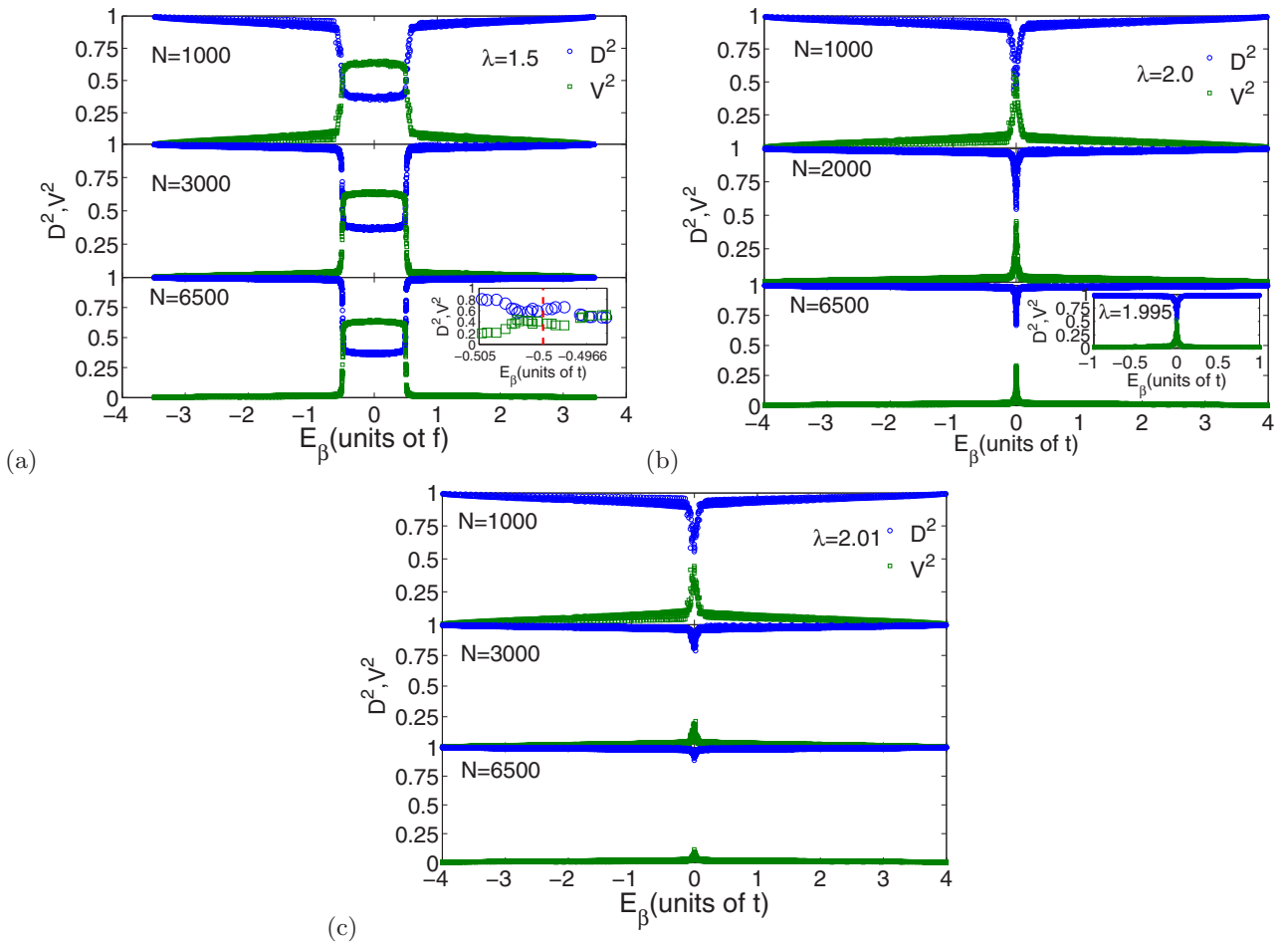

FIG. 3. For the SVP model, D^2 (blue symbols) and V^2 (green symbols) as functions of E_β for lattice sizes $N = 1000$, 3000, and 6500, respectively. (a) $\lambda = 1.5$, (b) $\lambda = 2.0$, and (c) $\lambda = 2.01$. Inset in (a): Partial enlarger for E_β near -0.5; the red line is for the function $E_\beta = -0.5$. Inset in (b): $\lambda = 1.995$.

$E_c = \pm(2.0 - \lambda)$ provided that $\lambda < 2.0$. Extended states are in the middle of the band ($|E| < 2.0 - \lambda$) and localized states are at the band edge ($2.0 - \lambda < |E| < 2.0 + \lambda$). For $\lambda > 2.0$, all states are localized.

For the on-site potential ε_i in the model, we set $\pi\alpha = 0.2$ and $\upsilon = 0.7$, which is the same as in Refs. [33–35]. We plot the distinguishability D^2 and visibility V^2 versus eigenenergies E_β in Figs. 3(a)–3(c) at $\lambda = 1.5$, 2.0, and 2.01, respectively. Here, lattice sizes $N = 1000, 3000$, and 6500 are used as examples. Figure 3 shows, similarly to Fig. 2(a), that due to the finite-size effect, for some states the relation $D^2 < V^2$ becomes $D^2 > V^2$ as the lattice size increases. These states are localized in the relatively larger lattice system. In what follows, we discuss only the result for $N = 6500$. Figure 3(a) shows that there is a crossover at $E_\beta^{\rm cr} \approx \pm 0.4966$ between the two curves for D^2 and V^2 versus E_β. As the relation $D^2 + V^2 = 1$ always holds, at the crossover point $D^2 = V^2 = 0.5$. It also shows that when $|E_\beta| < |E_\beta^{\rm cr}|$, $D^2 < V^2$; i.e., there are fewer particlelike properties than wavelike ones. For other E_β, $D^2 > V^2$; i.e., there are more particlelike properties than wavelike ones. In the case $\lambda = 1.5$, the ME value of MEs $E_c = \pm 0.5$, which is shown by the red line in the inset in Fig. 3(a). The inset shows that $E_\beta^{\rm cr}$ is a little less than E_c. Varga *et al.* have found that power-law decaying states appear close to the ME on the "metallic" side [40]. Such power-law decaying states are localized in lattices of infinite sizes. Our results agree with their finding. The inset in Fig. 3(b) shows that for $\lambda^* = 1.995$, $D^2 = V^2$ as E_β nears 0. For the same reason just mentioned [40], λ^* is not exactly equal to 2.0. For $\lambda > \lambda^*$, we find that $D^2 > V^2$ for all states. The result for $\lambda = 2.01$ as an example is shown in Fig. 3(c). In that situation, there are more particlelike properties than wavelike ones.

IV. DISCUSSION AND CONCLUSIONS

For the Harper and the SVP models, the Shannon information entropy in position space and that in momentum space have been provided to distinguish delocalized, localized, and critical states [26]. At the same time, the inverse participation ratio in phase space has been studied for the Harper and the Anderson models [41–43]. It was found that some important features of quantum states remain observable in phase space, while they may be lost in position or momentum space. These studies shed light on Anderson transitions. The corresponding results agree with the traditional conclusions [29–35]. The Shannon information entropy and the inverse participation ratio are one-site-averaged quantities, while the distinguishability D^2 and the visibility V^2 are two-site-averaged quantities. In other words, D^2 and V^2 take into account the correlation of wave functions on different lattice sites. Here, our results also support the points taken by some works from different perspectives [36–39]. In this sense, we give another view of existing discrepancies for these models.

On the other hand, the wave-particle duality is an important principle in quantum theory. According to the fringe visibility in a two-way single-photon interferometer, the inequality $D^2 + V^2 \leqslant 1$ has been derived to quantify the wave-particle duality, where D is the distinguishability and V is the visibility. Inspired by it, we adapt them to measure a single electron's particlelike and wavelike behaviors, respectively. We numerically calculated D^2 and V^2 for eigenstates in three well-known 1D lattice systems, i.e., the Anderson, the Harper, and the SVP models. The relation $D^2 + V^2 = 1$ always holds. In combination with existing results on the electronic localization properties in the three models, we have found that $D^2 < V^2$, $D^2 = V^2$, and $D^2 > V^2$ for delocalized, critical, and localized states, respectively. In this sense, the Anderson transition can be viewed as a transition from relatively more particlelike properties to relatively more wavelike ones, which supports the conclusions in Refs. [1–3]. In fact, the transition of a quanton from a particle to a wave nature is a fundamental and unsolved subject. Our study has perhaps shed further light on it.

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